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Numerical simulation of particle transport in the boundary layer with implications for SARS-CoV-2 virions distribution in urban environments

Alexander Varentsov^{1,2,3}, Victor Stepanenko^{1,2,3}, and Evgeny Mortikov^{2,3}

¹Department of Meteorology and Climatology, Faculty of Geography, Lomonosov Moscow State University, Moscow, Russia

²Moscow Center of Fundamental and Applied Mathematics, Moscow, Russia

³Research Computing Center, Lomonosov Moscow State University, Moscow, Russia

This paper presents the development and application of a numerical Lagrangian model of the transport of aerosol particles in the urban boundary layer of the atmosphere with a high spatial resolution. The development of the model is motivated by the limited measurement methods for observing aerosol concentrations in urban environments, both in terms of coverage density and in terms of accuracy and representativeness. The growing interest of the world community in the problems of monitoring air pollution in cities and the atmospheric distribution of biologically active aerosols also became a motivating factor.

The model uses the equation of motion to calculate the trajectory of a particle suspended in the air. It is based on Newton's second law and takes into account the forces of gravity, buoyancy and air resistance. The influence of stochastic turbulent eddies on the particle motion is taken into account in the model by using turbulent parameterizations. The effect of turbulence is important when describing the motion of particles in this model, since aerosols have a size much smaller than the grid step of the input data and can stay inside one cell for a long time, being under the influence of subgrid vortices. In this model, three parameterizations are implemented: a simple Gaussian model, a random displacement model, and a random walk model. In all three, the pulsation velocity component is a normally distributed random variable, but in the first two parameterizations it is generated at each time step of the Lagrangian model. In the last one, the interaction time of the particle with the turbulent vortex is introduced, during which the pulsation velocity component acting on the particle remains constant, characterizing the effect of a particular vortex. Additionally, a version of the model based on the Langevin equation has been implemented to more accurately account for the effect of turbulence on particle motion.

The developed numerical model is implemented in a program code in the C++ programming language and allows one to calculate individual trajectories of motion and concentrations of particles. Input data (wind speed components, turbulence characteristics and others) can be set analytically or imported from hydrodynamic models.

The model has been successfully tested and verified on several idealized analytical solutions – an

equivalence is obtained in terms of the concentration field. Experiments have also been carried out to reproduce the transport of particles in a series of urban canyons, including particles with a finite half-life that simulate the COVID-19 virions (SARS-CoV-2). Based on the results of the calculations, the influence of stratification, particle size and lifetime on the transport of aerosols in a typical urban environment was estimated.

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